

A simple model for magnetism in itinerant electron systems

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Abstract

A new lattice model of interacting electrons is presented. It can be viewed as a classical Hubbard model in which the energy associated to electron itinerance is proportional to the total number of possible electron jumps. Symmetry properties of the Hubbard model are preserved. In the half-filled band with strong interaction the model becomes the Ising model. The main features of the magnetic behavior of the model in the one-dimensional and mean-field cases are studied.

Key words: Classical spin model, Lattice model, magnetism

1 Introduction

The Heisenberg model[1] expresses the energy dependence of localized electron spins by means of the exchange interaction. This assumption creates a starting point for an analysis on magnetic states in insulators. There are a few well founded results for this model. For instance, one-dimensional systems, the Bethe ansatz and bosonization solutions provide a set of exact solutions of the model[2]. Rigorous results at zero temperature have been obtained for two and three hypercubic lattices[3]. By numerical approach, physical properties are exact results for finite systems and have been conjectured as an exact result for the properties of infinite systems[4]. More generally, the study of the Heisenberg model is made using methods of approximated solutions. However, these approaches certainly contain partial information that can differ from the exact solution. Another natural possibility is to introduce a new model that makes the analytical analysis easier or that can evidently be solved exactly. It is important, however, that the model remains appropriate for describing magnetic systems. This picture can be emphasized considering the Ising model[5] which is the most important simplification of the Heisenberg model.

The crucial assumption is that the Ising Hamiltonian is explicitly diagonal, but nontrivial from the point of view of statistical mechanics.

The Ising model has played a key role in the development of the theory of interacting systems. It has a phase transition at finite temperature that can be worked out with mathematical rigor and yields an exact solution in two dimensions. Although it has only been considered a theoretical model for many years, experiments have brought forth evidence of its applicability for real magnetic materials (see [6] and references therein). It should be noted that another virtue of the model is its correspondence with systems such as lattice gases, binary alloys and neural networks among others[7].

In conductors, the study of magnetism is more complex because the electrons of magnetic states are often not localized. The basic model to describe the interaction between electrons having translational degrees of freedom is the Hubbard model[8].

Suggested in 1963, the Hubbard model also much like the Heisenberg model remains with many of its basic features in debate. An important problem to be answered is to establish which limits within the parameters of the Hubbard model that favor ferromagnetism when neither the electronic interaction nor the electronic itinerance favors this situation. Many believe that ferromagnetism can only be observed when there are more than one electronic orbital per site. In the simple Hubbard model when only one orbital per site is present the induced antiferromagnetism due to the electronic itinerant term disfavors ferromagnetism. However, in the extreme limits of electronic repulsion and in special lattice cases, we can find ferromagnetism in this model[9]. Indeed, the small number of accurate solutions (one-dimensional systems, ground state theorems and numerical approach)[10,11] and the difficulty of studying the Hubbard model indicate that the understanding of this problem remains vague. For example, we do not have an accurate solution for the transition metals.

Knowing the difficulties in dealing with the Hubbard model and the importance of studying the effect of the electronic itinerance term, I will shortly introduce a model that remains with the essential features of the Hubbard model, but simplifies it using a classical situation for the hopping. Despite the simplification, this model must be capable of describing the magnetism of materials with itinerant electrons. This paper is organized as follows. In Sec. 2 the model is described. The one-dimensional ring considering nearest-neighbor hopping is solved in Sec. 3. Sec. 4 presents the mean-field solution for the model. Sec. 5 is devoted to conclusions.

2 Model

The starting point for the present model is the Hubbard model, which has the following Hamiltonian

$$\mathfrak{H} = - \sum_{ij\sigma} t_{ij} a_{i\sigma}^\dagger a_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

where $a_{i\sigma}^\dagger$, $a_{i\sigma}$ are the creation and annihilation operators for electrons of spin σ at site i . The density of electrons is denoted by $n_\sigma = \frac{1}{N} \sum_i n_{i\sigma}$ where N is the number of lattice sites, and $n_{i\sigma} = a_{i\sigma}^\dagger a_{i\sigma}$ is the number operator for electrons of spin σ at site i . The first term of the Hamiltonian corresponds to the hopping of the electrons between sites i and j , and t_{ij} is the hopping integral representing the overlap of electron wave functions. Usually, the overlapping is assumed only over nearest neighbour sites. The second term represents the on-site Coulomb interaction (U) between the electrons.

The crucial ingredient for the construction of the model is to consider the energy associated to the electron itinerance as being equal to the total number of possible electron jumps. Hence, it is easy to see that the Hamiltonian can be defined as

$$\mathfrak{H} = - \sum_{ij\sigma} t_{ij} n_{i\sigma} (1 - n_{j\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (2)$$

In this case, the hopping term commutes with the Coulombic term. The states of the number operator are eigenstates of the Hamiltonian. As in the Ising model, the Hamiltonian is explicitly diagonal and the model is much easier to study compared to the Hubbard model.

The Hamiltonian of Eq. (2) can be seen as an approximation of the extended Hubbard model, constructed by the inclusion of a third term in the simple Hubbard model (Eq. 1) which describes the off-site Coulomb repulsion between electrons[12],[13],[14]. The off-site interaction has been appropriate for compounds that exhibit near-neighbors interaction compared to the bandwidth, in particular quasi one-dimensional organic conductors[13]. The Hamiltonian of Eq. (2) is the zero-band-width limit of the extended Hubbard model assuming off-site interaction only between electrons of equal spins. This assumption can be justified considering that the electron repulsion of different spins has its main contribution on the same site, while electron repulsion of equal spins contributes only to different sites by the Pauli exclusion principle. Hubbard showed that the zero-band-width limit of the one-dimensional extended Hubbard model can present an interpretation of the optical spectra of many tetracyanoquinodimethane salts. Indeed, some features of finite

bandwidth may well survive in the present model if the interaction effects are of dominant importance[13]. These considerations indicate to be reasonable the application of the model represented by the Hamiltonian of Eq. (2) to the quasi one-dimensional organic conductors as well as to other materials with the same electronic structure.

Since we wish a model capable of describing the magnetic properties of materials with itinerant electrons, it should be important to observe that relevant symmetry transformations of the Hubbard model are preserved, such as the U(1) charge symmetry and the particle-hole transformation in the case of bipartite lattice. Notice that this has an important consequence: the condition for the chemical potential $\mu = U/2$ for the half-filled band, independently of the temperature, is identical to that of Hubbard model. It is also crucial to observe the ground state configurations of the new model. Here, only general features will be presented. Detailed analyses depend on specific works using this model. It is easy to see that at half-filled band the two Néel antiferromagnetic configurations are ground states of the new Hamiltonian for $U > 0$ in non frustrated lattices. When the number of electrons is smaller than half of the number of lattice sites the ground state becomes highly degenerate and the ferromagnetic configuration has also the lower energy. The model favors the antiferromagnetic order, but for low or high electron densities there is a tendency towards the coexistence of ferromagnetism with antiferromagnetism. As will be observed in the one-dimensional case, for the half-filled band the antiferromagnetic ordered phase exists only at zero temperature. With finite temperature the ordered phase does not exist.

In the square lattice, for the half-filled band case, the ground state is antiferromagnetic, but at finite temperature(T) the solution has not yet been found. For this same lattice, the Hubbard model is not solvable and even its ground state is not known. Using the Monte-Carlo approach, Hirsch[11] predicts antiferromagnetic ordered ground state only at $T = 0$. I believe that both the new model and the Hubbard model yield a similar result to the relation between the Ising and Heisenberg models. With finite temperature, both the new and the Ising models have an ordered phase while the Hubbard and the Heisenberg models do not[15].

3 One-dimensional solution

One sees that in this case the Hamiltonian (2) can be written as $\mathcal{H} = \sum_i E_i$, where

$$E_i = t(n_{i\uparrow}n_{i+1\uparrow} + n_{i\downarrow}n_{i+1\downarrow}) + Un_{i\uparrow}n_{i\downarrow} - t(n_{i\uparrow} + n_{i\downarrow}). \quad (3)$$

Let us take $t_{ij} = t > 0$ over nearest neighbor sites, otherwise $t_{ij} = 0$. The thermodynamic properties of the model can be obtained using the transfer matrix method. The grand-canonical partition function, at temperature T , is written as $Z = \sum_i \lambda_i^N$, where λ_i are eigenvalues of the transfer matrix

$$\widehat{X}_{i,i+1} = e^{-(E_i - \frac{\mu}{2} \sum_{\sigma} (n_{i\sigma} + n_{i+1\sigma})) / k_B T}, \quad (4)$$

where rows and columns are labelled by $n_{i\sigma}$ and $n_{i+1\sigma}$, respectively. The matrix \widehat{X} is 4x4 and will be numerically diagonalized. The largest eigenvalues λ_{\max} of \widehat{X} are found. Considering the thermodynamic limit ($N \rightarrow \infty$), the free energy is $A/N = -k_B T \ln \lambda_{\max}$, and the thermodynamic properties follow from properly differentiating the free energy. For the half-filled band the analytical expression for λ_{\max} is

$$\lambda_{\max} = \frac{(1+y)(1+w) + \sqrt{(1+y^2)(1+w)^2 - 2y(1-6w+w^2)}}{2wy}, \quad (5)$$

where $w = \exp[-2t/(k_B T)]$ and $y = \exp[-U/(2k_B T)]$. Figure 1 presents the specific heat C as a function of temperature for typical values of U/t for the half-filled band. For $U/t \leq 13.5$ it has a peak. Whose value increases with U/t until the maximum $C/Nk_B = 1.38$ for $U/t = 0.7$ and decreases for larger values of U/t . For $U/t > 13.5$ the peak splits in two, which reflects a rearrangement of the fermionic structure in the system[16]. The picture presented is analogous to those ones of the one-dimensional half-filled band Hubbard[17] and Falikov-Kimball models[16]. However, the critical values of U/t which causes this splitting are different: $U/t = 0$ for the Falikov-Kimball model, $U/t = 4$ for the Hubbard model and $U/t = 13.5$ for the present model. For $U/t \rightarrow \infty$ the second peak (high-temperature peak) gets further from the first peak as $T \rightarrow \infty$, and then the first peak yields the specific heat with the maximum value of $C/Nk_B = 0.44$ which is exactly the specific heat of the Ising model[18]. Figure 2 shows the temperature dependence of the magnetic susceptibility χ for the several choices of U/t in the half-filled case. The χ has a maximum and vanishes at zero temperature. For large U/t the magnetic susceptibility is well described by the Ising model as was evidenced by the specific heat in Fig. 1. Finally, it is obtained without further difficulties no phase transition at any finite T and no long-range order for all $T > 0$.

4 Mean-field solution

Having obtained solutions for the one-dimensional case one presents below the mean-field solution. The self-consistent equations for translationally invariant

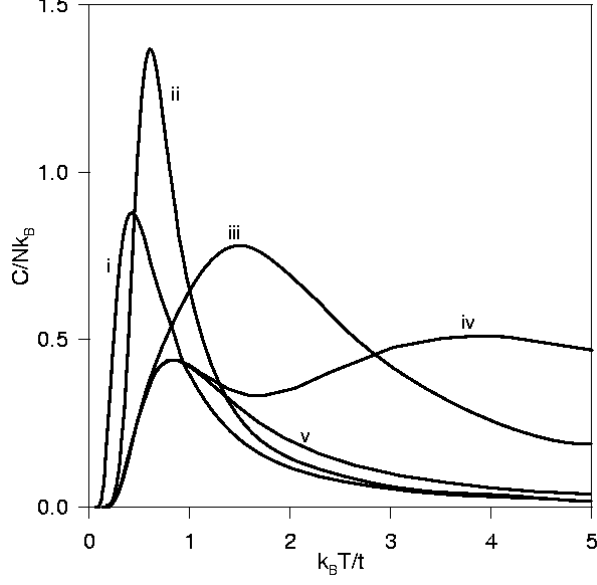


Fig. 1. Specific heat C/Nk_B of infinite chain versus temperature for typical values of U/t : i) $U/t = 0$; ii) $U/t = 1$; iii) $U/t = 8$; iv) $U/t = 20$; v) $U/t \rightarrow \infty$.

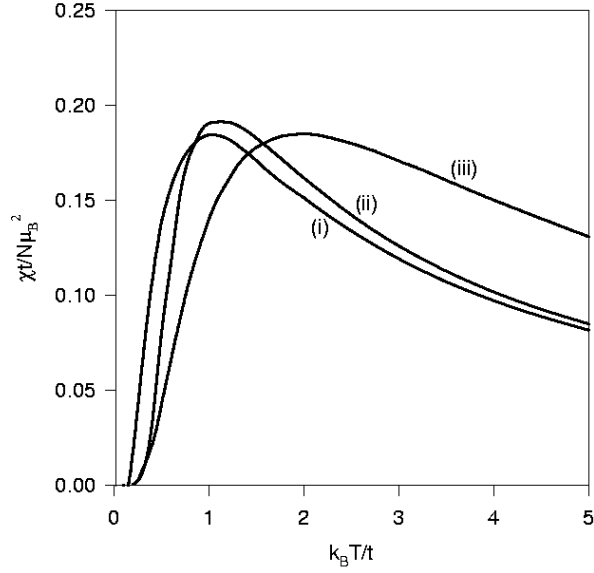


Fig. 2. Magnetic susceptibility of infinite chain versus temperature for typical values of U/t : i) $U/t = 0$; ii) $U/t = 1$; iii) $U/t = 32$.

systems are given by

$$n = \frac{2 \cosh \left(\beta \left(\frac{mtz}{2} - h \right) \right) e^{\beta(\mu+tz(1-n)/2)} + 2e^{\beta(2\mu-U)} e^{\beta tz(1-n)}}{1 + 2 \cosh \left(\beta \left(\frac{mtz}{2} - h \right) \right) e^{\beta(\mu+tz(1-n)/2)} + e^{\beta(2\mu-U)} e^{\beta tz(1-n)}} \quad (6)$$

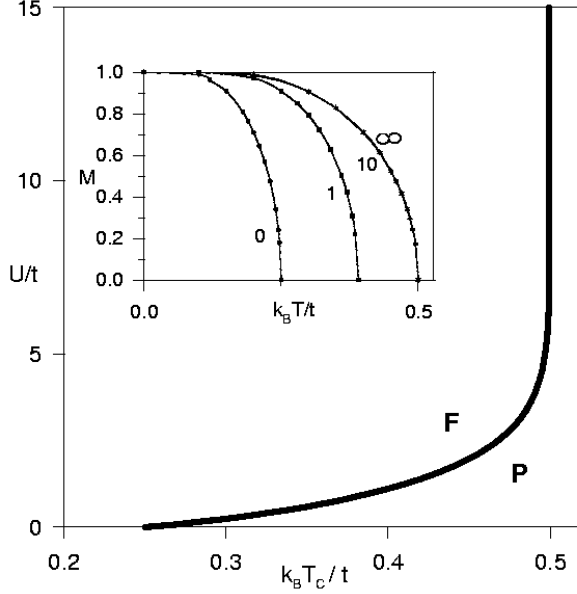


Fig. 3. Phase diagram for the ferromagnetic (F) and paramagnetic(P) states of the model in the half-filled band. The inset shows the temperature dependence of the magnetization. The numbers denote the U/t values.

and

$$m = \frac{2 \sinh \left(\beta \left(\frac{mtz}{2} - h \right) \right) e^{\beta(\mu+tz(1-n)/2)}}{1 + 2 \cosh \left(\beta \left(\frac{mtz}{2} - h \right) \right) e^{\beta(\mu+tz(1-n)/2)} + e^{\beta(2\mu-U)} e^{\beta tz(1-n)}} \quad (7)$$

where n and m are the mean values of the electron number ($n = \langle n_i \rangle = \langle \sum_{i\sigma} n_{i\sigma} \rangle$) and local magnetization ($m = \langle m_i \rangle = \langle \sum_i (n_{i\uparrow} - n_{i\downarrow}) \rangle$), respectively, on a lattice where each site has z nearest neighbours. In the half-filled band $n = 1$, which implies that $\mu = U/2$ independently of the temperature and it is easy to see that $m = \left[\coth \left(\beta \left(\frac{mtz}{2} - h \right) \right) + e^{-\beta U/2} \right]^{-1}$. The dependence of the magnetization on U/t is considered. The critical temperature T_c is (assuming $k_B = 1$, $zt = 1$)

$$U = -2T_c \ln \left(\frac{1 - 2T_c}{2T_c} \right). \quad (8)$$

The phase diagram is shown in Fig. 3. Below T_c there is a spontaneous magnetization. The inset in Fig. 3 shows the temperature dependence of the magnetization. The magnetization increases with decreasing temperature and attains the saturate value at zero temperature. Mean-field solutions suggest that the magnetic order phase increases if U/t increases in agreement with the Hubbard model predictions[11].

Notice that for the $U = 0$ limit the model is reduced to a lattice gas of two types of atoms. This means that the present model can also be interpreted as a generalization of the Ising model which is exactly the $U/t \rightarrow \infty$ case.

5 Conclusions

In summary, a classical lattice model was introduced to describe the magnetism of itinerant electron systems. It is much easier to analyze than the Hubbard model. I have illustrated some features of its magnetic properties. These general results clearly show that the presented model can be viewed as a classical Hubbard model in the same way as the Ising model can be considered with relation to the quantum Heisenberg model. Naturally, it is not able to capture the quantum frustration of the Hubbard model much like the Ising model cannot capture the quantum frustration of the Heisenberg model. However, I believe that it is a promising help to qualitatively clarify our understanding on the nature of magnetism. In addition, the proposed model is a generalization of the Ising model. The possibility of generalizing the Onsager solution for the square lattice case would be useful in future phase transition research.

6 Acknowledgements

I thank M. E. de Souza and A. Reikdal for reading the manuscript. This work was financially supported by CNPq and FAP-SE.

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